pH-metric Result

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)   -4.20   ±1.91 (n=49)
logP (neutral X)   3.81   ±0.01 (n=49)

18C-03013 Points 1 to 30

M12_octanol concentration factor   0.900
Carbonate   0.0742 mM
Acidity error   -0.41736 mM

18C-03013 Points 31 to 56

M12_octanol concentration factor   0.766
Carbonate   0.1690 mM
Acidity error   0.13861 mM

18C-03013 Points 57 to 80

M12_octanol concentration factor   1.090
Carbonate   0.1802 mM
Acidity error   -0.94352 mM

Warnings and errors

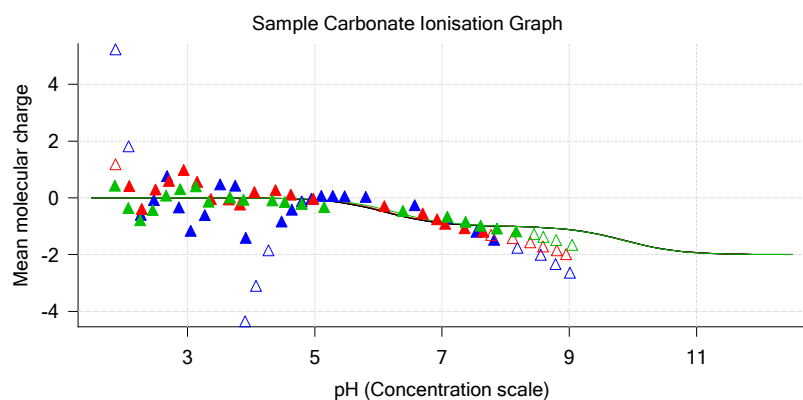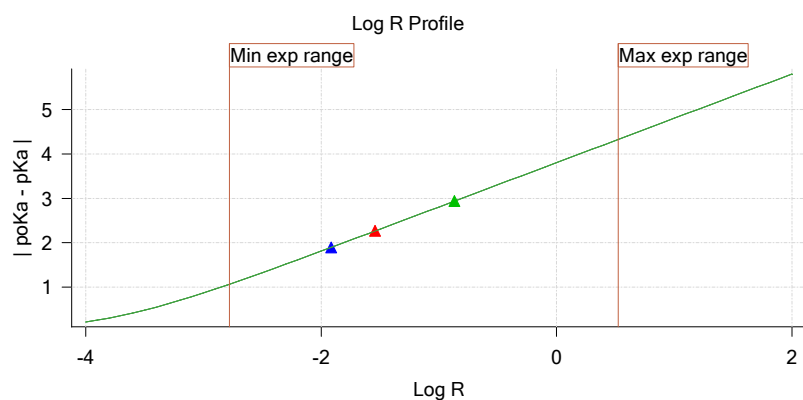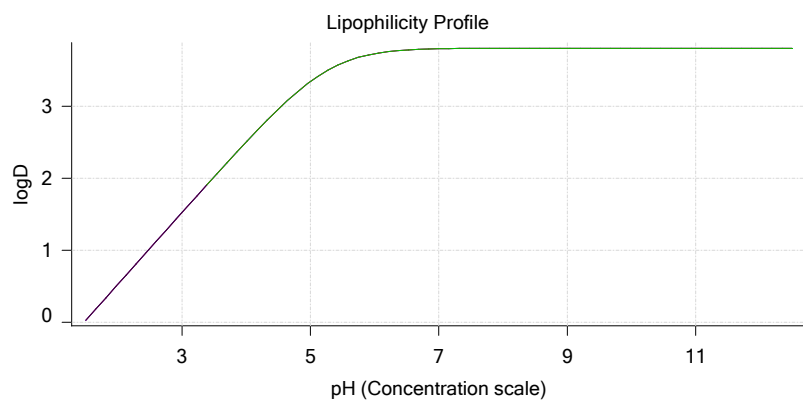Errors   None
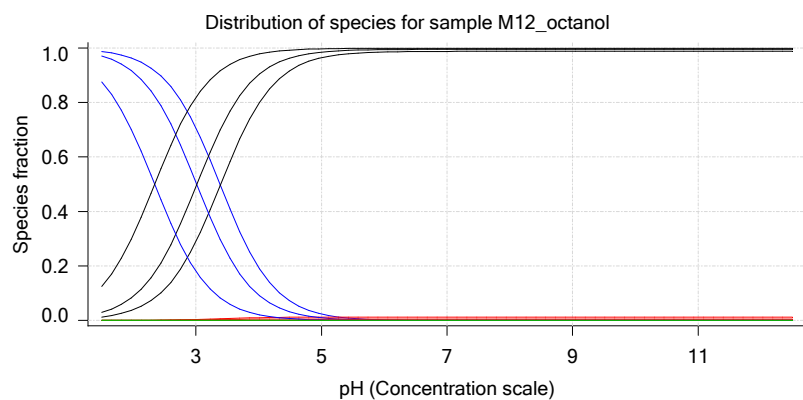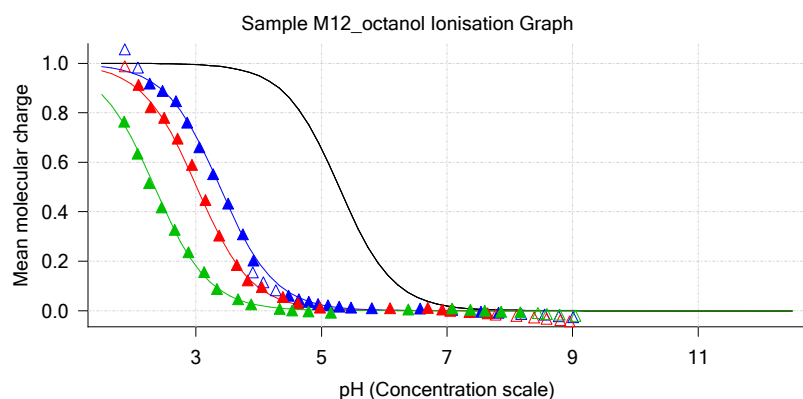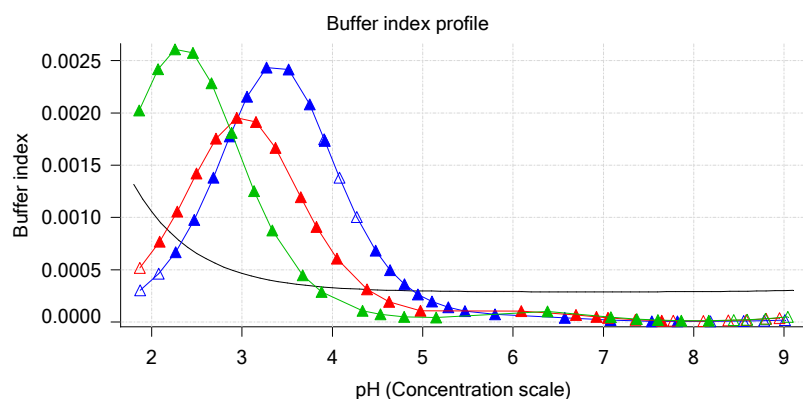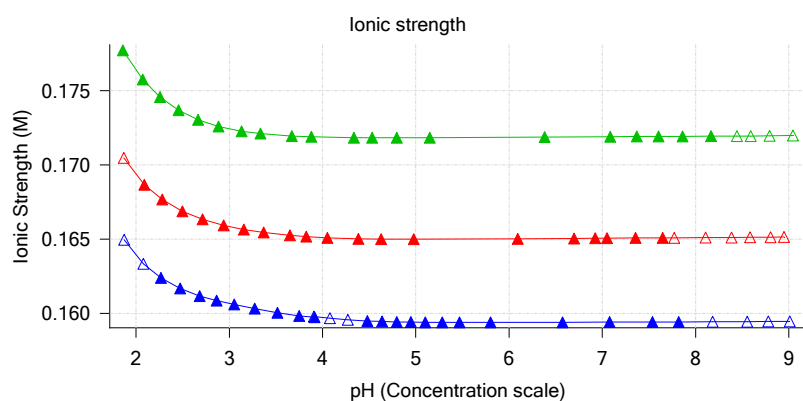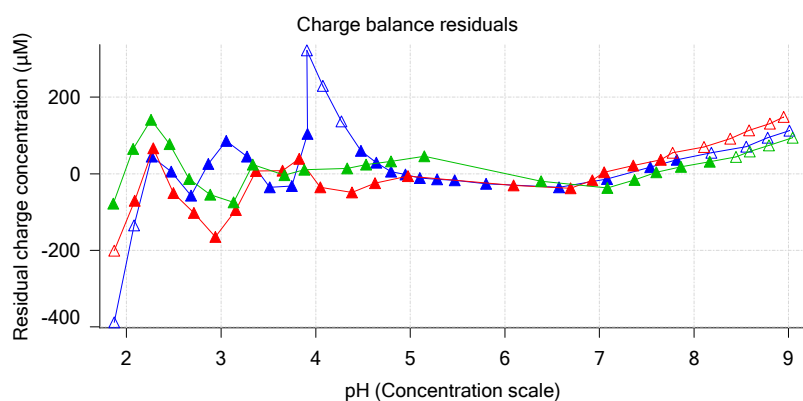Warnings   One or more logP values out of range

Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	-0.47	74.87 %	0.00 %	0.00 %	25.12 %	
1.200	-0.27	65.28 %	0.01 %	0.00 %	34.71 %	Stomach pH
2.000	0.53	22.96 %	0.01 %	0.00 %	77.03 %	
3.000	1.52	2.89 %	0.02 %	0.00 %	97.09 %	
4.000	2.50	0.30 %	0.02 %	0.00 %	99.69 %	
5.000	3.34	0.03 %	0.02 %	0.00 %	99.95 %	
6.000	3.73	0.00 %	0.02 %	0.00 %	99.98 %	
6.500	3.78	0.00 %	0.02 %	0.00 %	99.98 %	
7.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	
7.400	3.80	0.00 %	0.02 %	0.00 %	99.98 %	Blood pH
8.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	
9.000	3.81	0.00 %	0.02 %	0.00 %	99.98 %	
10.000	3.81	0.00 %	0.02 %	0.00 %	99.98 %	
11.000	3.81	0.00 %	0.02 %	0.00 %	99.98 %	
12.000	3.81	0.00 %	0.02 %	0.00 %	99.98 %	

pH-metric Result

Sample name: **M12_octanol**　　　　　　　　Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP**　　　　　Analyst: **Pion**
Assay ID: **18C-03013**　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M12_octanol Ionisation Graph

Distribution of species for sample M12_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

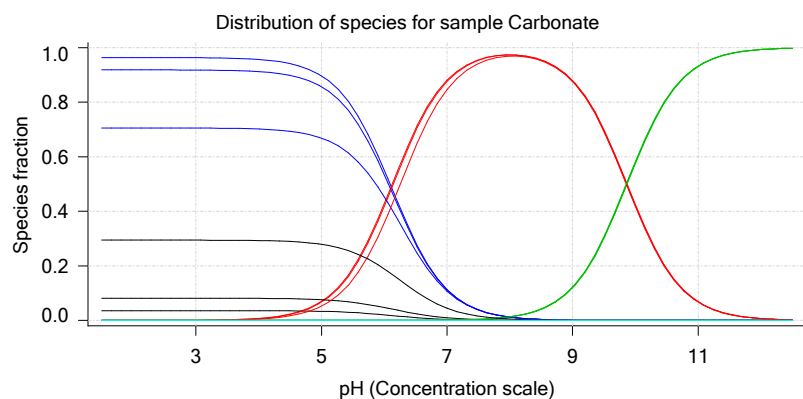Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-03013 Points 1 to 30

Overall results

RMSD   1.132
Average ionic strength   0.160 M
Average temperature   24.9°C
Partition ratio   0.0122 : 1
Analyte concentration range   4689.3 µM to 4859.4 µM
Total points considered   21 of 30

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

Alpha   0.111   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
S   0.9988   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
jH   1.0   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
jOH   -0.8   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl   0.999058   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH   0.999845   3/3/2018 4:33:34 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor   0.900
M12_octanol stoichiometry   1.000
Chloride stoichiometry   1.000
Base pKa 1   5.28
logP (XH +)   1.02
logP (neutral X)   3.87

Sample graphs

Ionisation of sample M12_octanol

Distribution of species for sample M12_octanol

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**
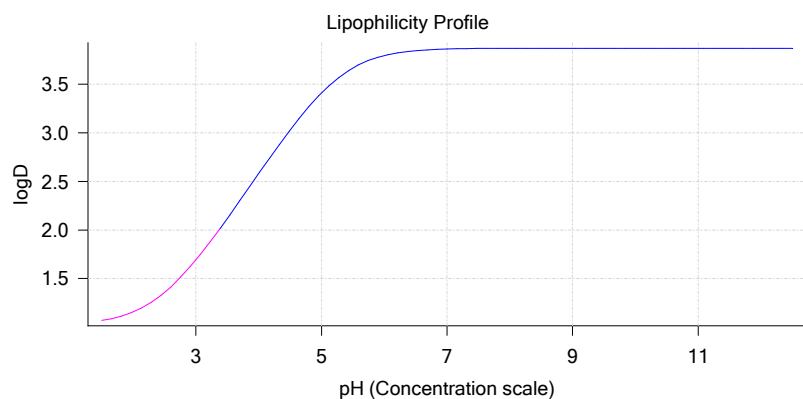
Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.04	88.32 %	0.00 %	11.25 %	0.42 %	
1.200	1.04	88.11 %	0.01 %	11.23 %	0.66 %	Stomach pH
2.000	1.16	85.08 %	0.04 %	10.84 %	4.03 %	
3.000	1.69	62.24 %	0.33 %	7.93 %	29.50 %	
4.000	2.58	16.89 %	0.89 %	2.15 %	80.07 %	
5.000	3.41	2.04 %	1.07 %	0.26 %	96.63 %	
6.000	3.80	0.21 %	1.09 %	0.03 %	98.67 %	
6.500	3.85	0.07 %	1.09 %	0.01 %	98.83 %	
7.000	3.86	0.02 %	1.09 %	0.00 %	98.88 %	
7.400	3.87	0.01 %	1.09 %	0.00 %	98.90 %	Blood pH
8.000	3.87	0.00 %	1.09 %	0.00 %	98.90 %	
9.000	3.87	0.00 %	1.09 %	0.00 %	98.90 %	
10.000	3.87	0.00 %	1.09 %	0.00 %	98.91 %	
11.000	3.87	0.00 %	1.09 %	0.00 %	98.91 %	
12.000	3.87	0.00 %	1.09 %	0.00 %	98.91 %	

Carbonate and acidity

Carbonate 0.074 mM
Acidity error -0.417 mM

Other graphs

Assay progress

Titration graph

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
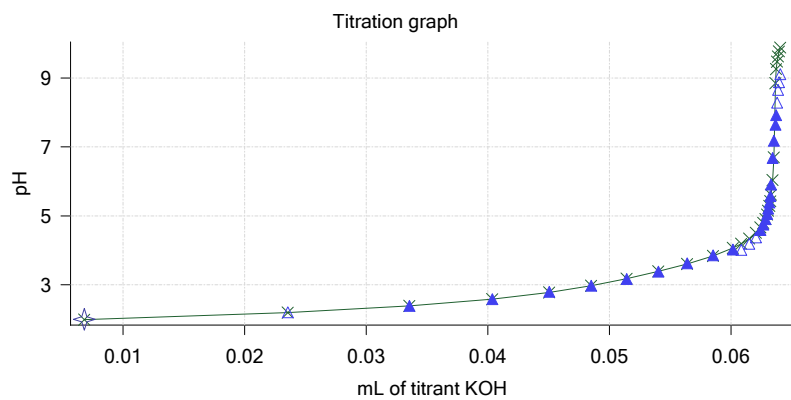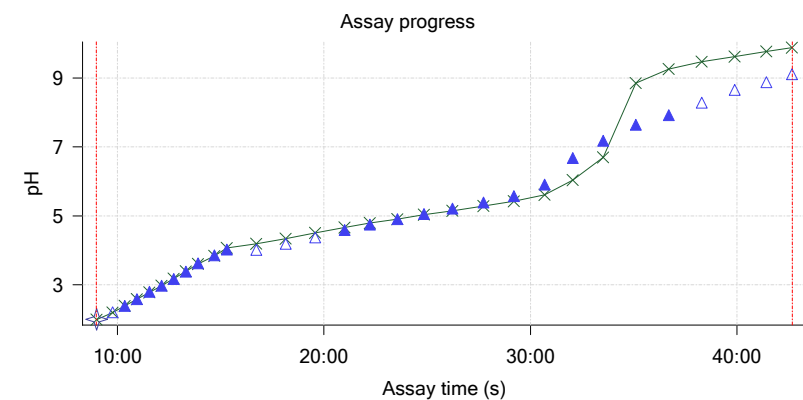Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Min exp range

Max exp range

Ionisation of sample Carbonate

6.11

9.87
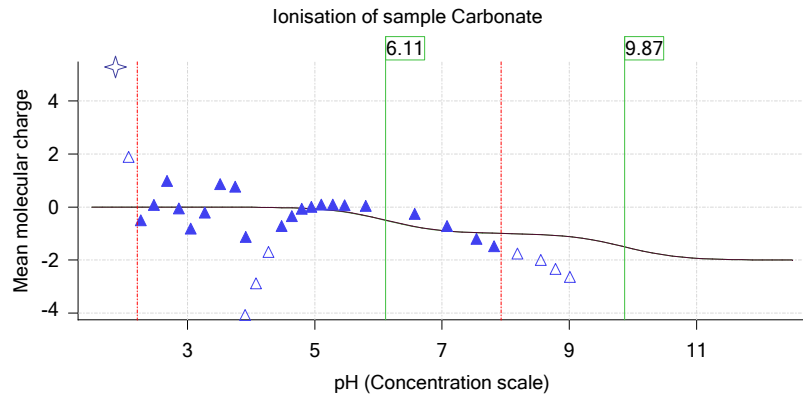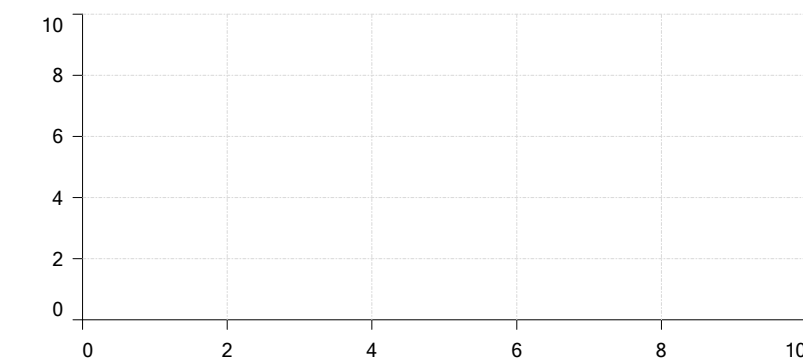
Sample name: **M12_octanol**   Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-03013**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 2 of 3   18C-03013 Points 31 to 56

Overall results

RMSD	0.588
Average ionic strength	0.165 M
Average temperature	25.0°C
Partition ratio	0.0288 : 1
Analyte concentration range	4305.5 µM to 4450.5 µM
Total points considered	19 of 26

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

🔒	Alpha	0.111	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	S	0.9988	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jH	1.0	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jOH	-0.8	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

🔒	0.50 M HCl	0.999058	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	0.50 M KOH	0.999845	3/3/2018 4:33:34 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔷	M12_octanol concentration factor	0.766
🔒	M12_octanol stoichiometry	1.000
🔒	Chloride stoichiometry	1.000
🔒	Base pKa 1	5.28
🔒	logP (XH +)	1.02
🔷	logP (neutral X)	3.88

Sample graphs

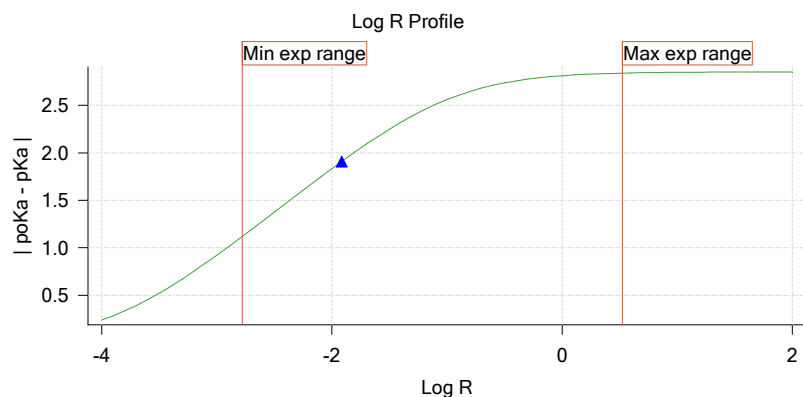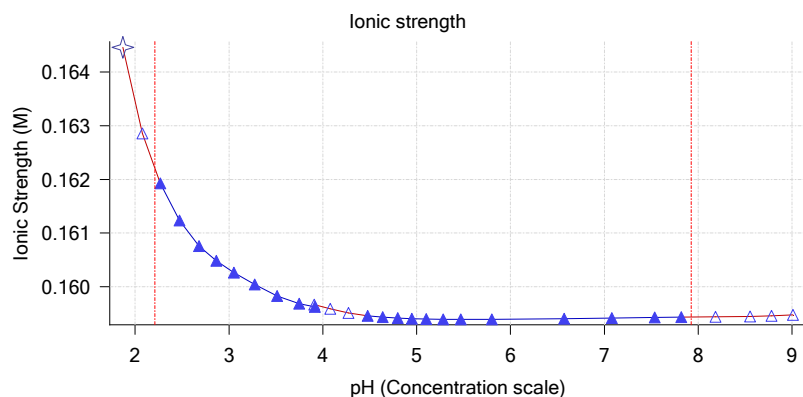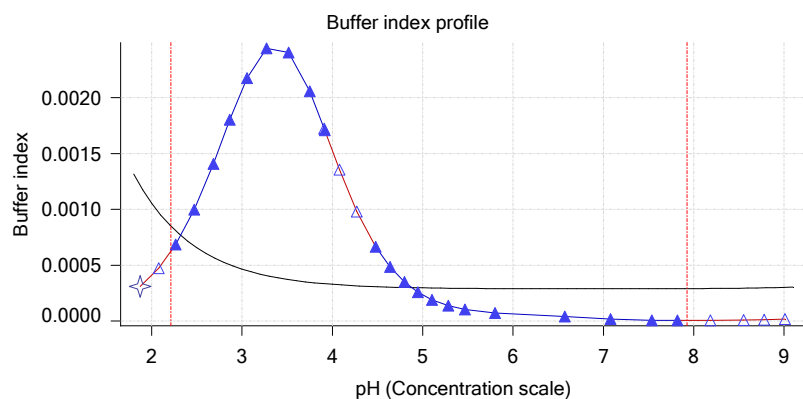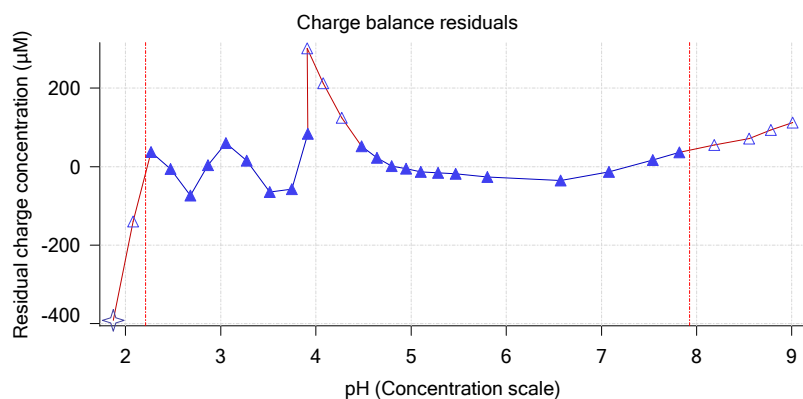Ionisation of sample M12_octanol

Distribution of species for sample M12_octanol

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

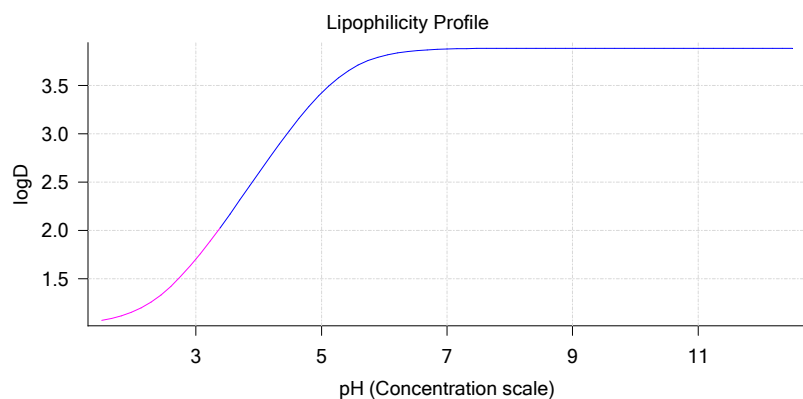| pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.04	76.18 %	0.00 %	22.94 %	0.88 %	
1.200	1.05	75.78 %	0.01 %	22.82 %	1.39 %	Stomach pH
2.000	1.16	70.56 %	0.04 %	21.25 %	8.16 %	
3.000	1.70	40.60 %	0.21 %	12.23 %	46.96 %	
4.000	2.59	7.74 %	0.41 %	2.33 %	89.52 %	
5.000	3.42	0.85 %	0.45 %	0.26 %	98.45 %	
6.000	3.81	0.09 %	0.45 %	0.03 %	99.44 %	
6.500	3.86	0.03 %	0.45 %	0.01 %	99.51 %	
7.000	3.88	0.01 %	0.45 %	0.00 %	99.54 %	
7.400	3.88	0.00 %	0.45 %	0.00 %	99.54 %	Blood pH
8.000	3.88	0.00 %	0.45 %	0.00 %	99.55 %	
9.000	3.88	0.00 %	0.45 %	0.00 %	99.55 %	
10.000	3.88	0.00 %	0.45 %	0.00 %	99.55 %	
11.000	3.88	0.00 %	0.45 %	0.00 %	99.55 %	
12.000	3.88	0.00 %	0.45 %	0.00 %	99.55 %	

Carbonate and acidity

Carbonate 0.169 mM
Acidity error 0.139 mM

Other graphs

Assay progress

Titration graph

Sample name: **M12_octanol** Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-03013** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
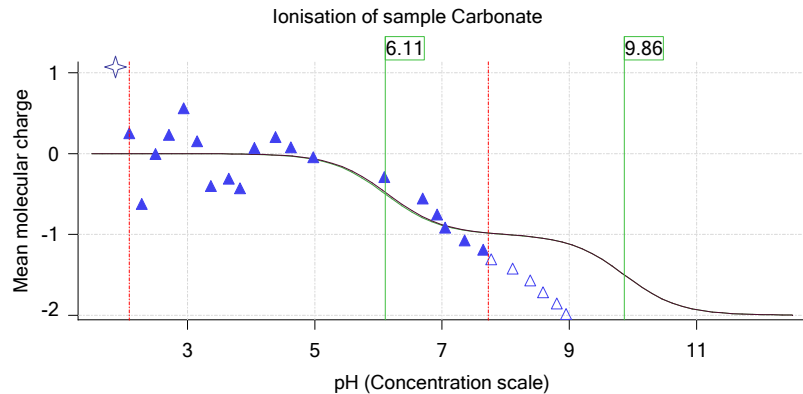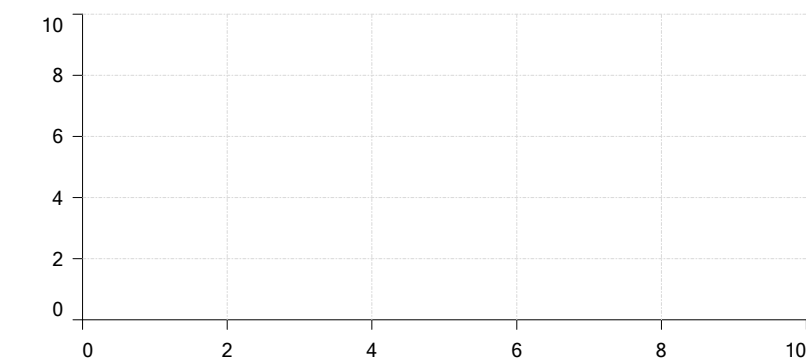
Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
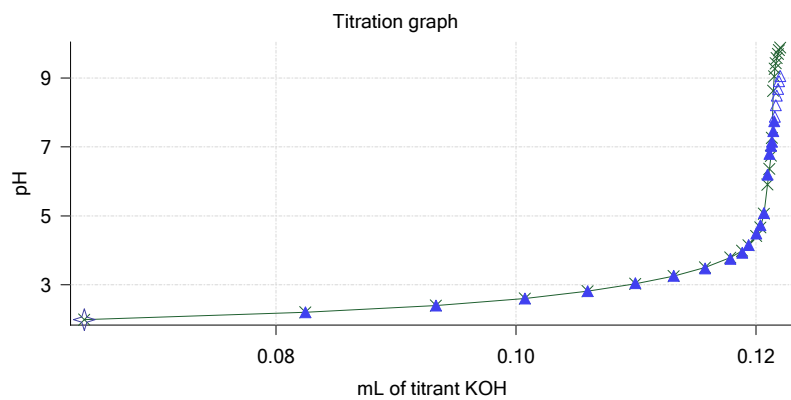Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-03013 Points 57 to 80

Overall results

RMSD   0.527
Average ionic strength   0.172 M
Average temperature   25.0°C
Partition ratio   0.1351 : 1
Analyte concentration range 3639.4 µM to 3752.4 µM
Total points considered   20 of 24

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

Alpha   0.111   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
S   0.9988   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
jH   1.0   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
jOH   -0.8   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl   0.999058   3/3/2018 4:33:34 PM   C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH   0.999845   3/3/2018 4:33:34 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor   1.090
M12_octanol stoichiometry   1.000
Chloride stoichiometry   1.000
Base pKa 1   5.28
logP (XH +)   1.02
logP (neutral X)   4.20

Sample graphs

Ionisation of sample M12_octanol

Distribution of species for sample M12_octanol

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
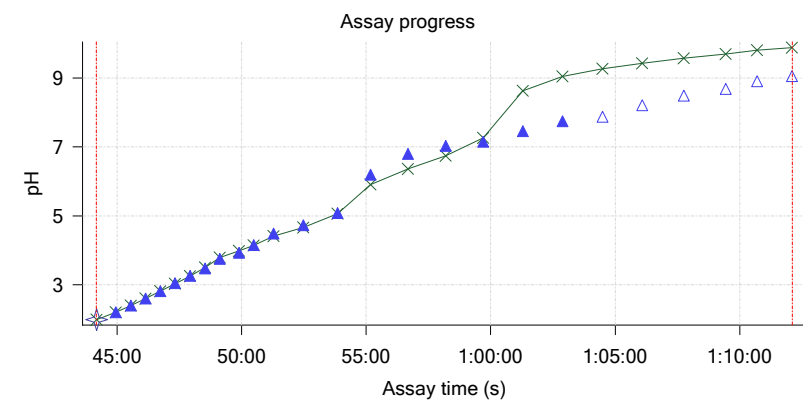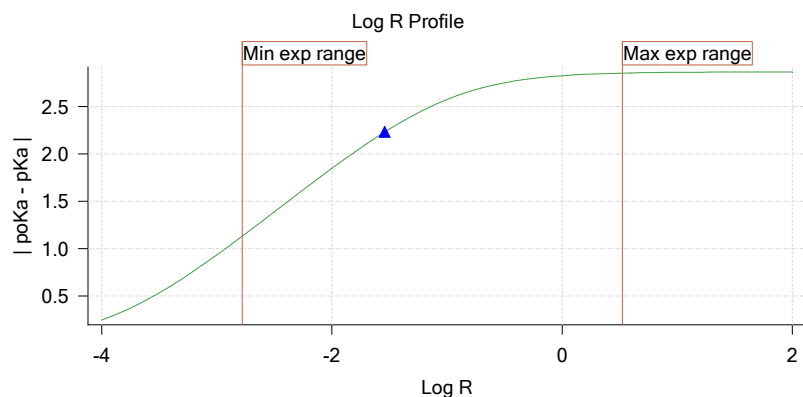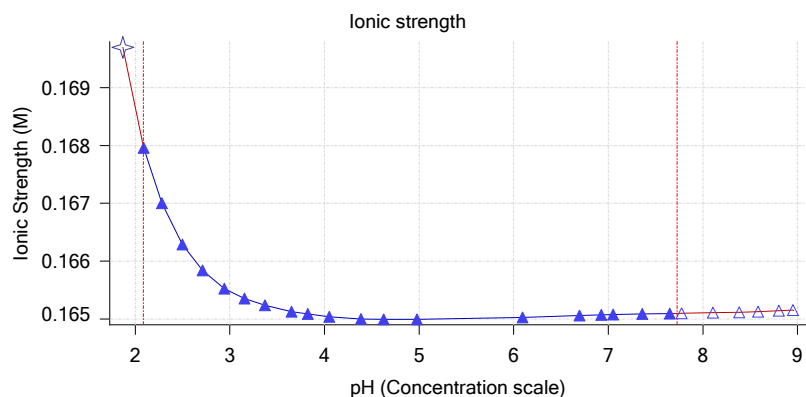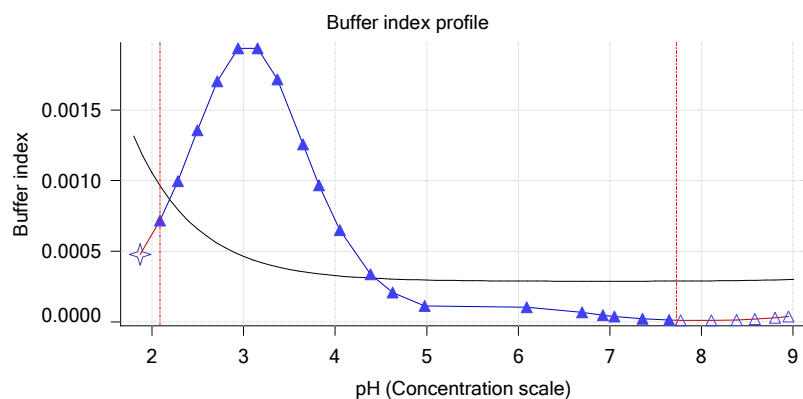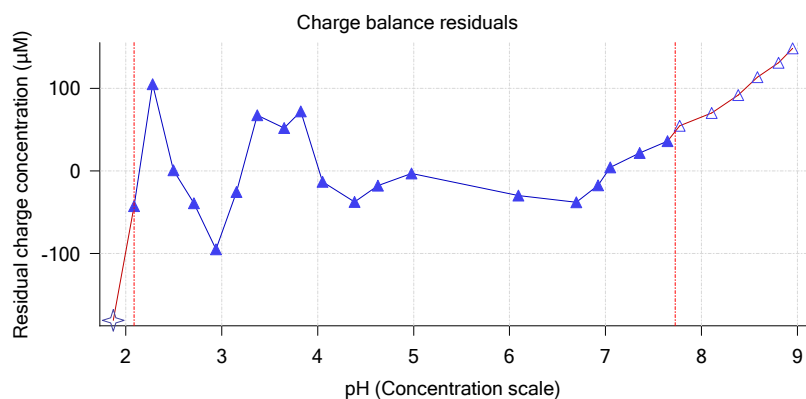Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
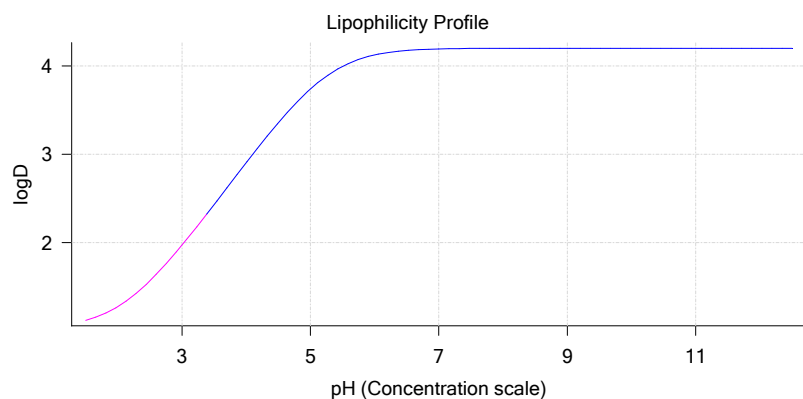
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.05	39.56 %	0.00 %	55.97 %	4.47 %	
1.200	1.07	38.55 %	0.00 %	54.54 %	6.90 %	Stomach pH
2.000	1.27	28.21 %	0.01 %	39.91 %	31.87 %	
3.000	1.97	7.29 %	0.04 %	10.31 %	82.36 %	
4.000	2.91	0.87 %	0.05 %	1.23 %	97.86 %	
5.000	3.74	0.09 %	0.05 %	0.12 %	99.74 %	
6.000	4.13	0.01 %	0.05 %	0.01 %	99.93 %	
6.500	4.18	0.00 %	0.05 %	0.00 %	99.95 %	
7.000	4.19	0.00 %	0.05 %	0.00 %	99.95 %	
7.400	4.20	0.00 %	0.05 %	0.00 %	99.95 %	Blood pH
8.000	4.20	0.00 %	0.05 %	0.00 %	99.95 %	
9.000	4.20	0.00 %	0.05 %	0.00 %	99.95 %	
10.000	4.20	0.00 %	0.05 %	0.00 %	99.95 %	
11.000	4.20	0.00 %	0.05 %	0.00 %	99.95 %	
12.000	4.20	0.00 %	0.05 %	0.00 %	99.95 %	

Carbonate and acidity

Carbonate   0.180 mM
Acidity error   -0.944 mM

Other graphs

Assay progress

Titration graph

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
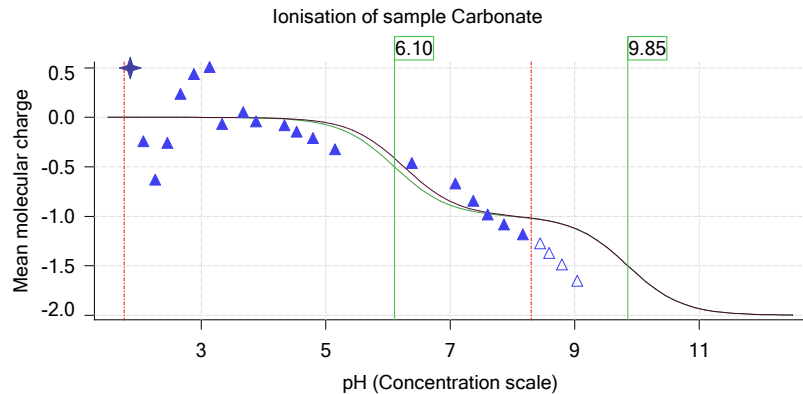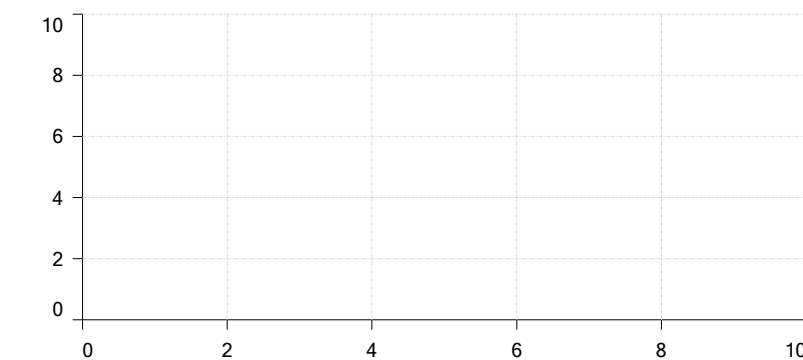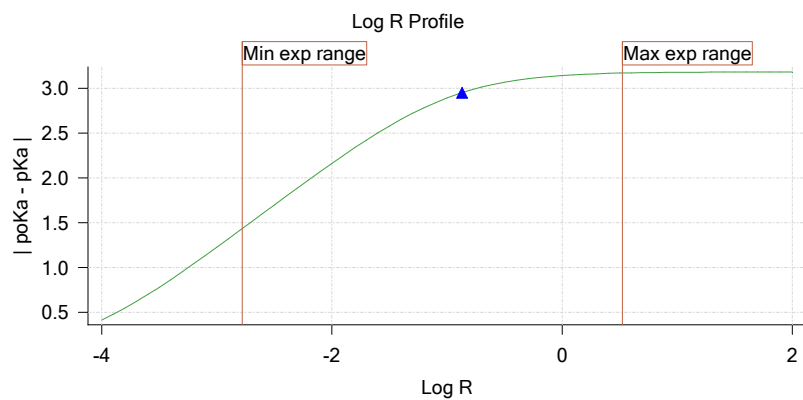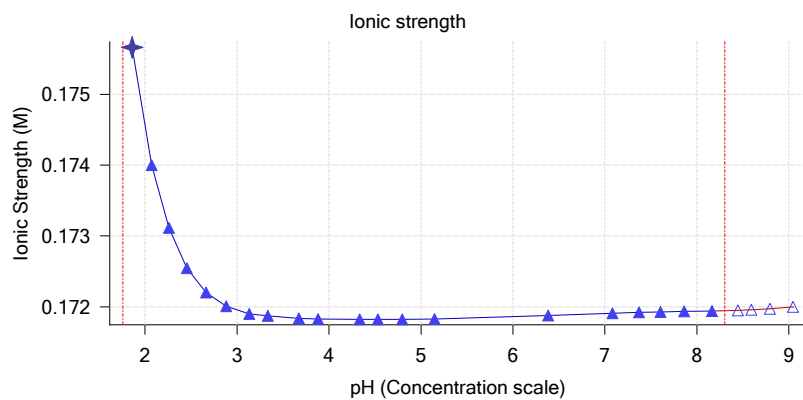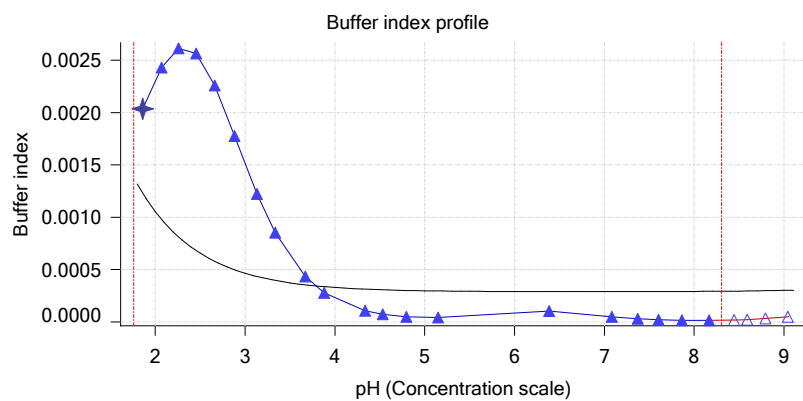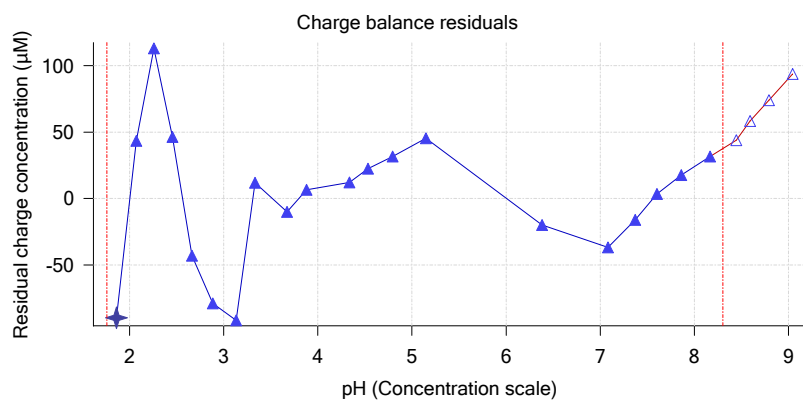
Sample name: **M12_octanol** Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-03013** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M12_octanol	2/28/2018 2:58:36 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.002240 g	3/2/2018 5:10:19 PM	User entered value
Formula weight	292.16 g/mol	2/28/2018 2:58:36 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	255.70	2/28/2018 2:58:36 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/28/2018 2:58:36 PM	User entered value
Sample is a	Base	2/28/2018 2:58:36 PM	User entered value
pKa 1	5.28	2/28/2018 2:58:36 PM	User entered value
logp (XH +)	1.02	3/2/2018 3:44:28 PM	User entered value
logP (neutral X)	3.79	3/2/2018 3:44:35 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

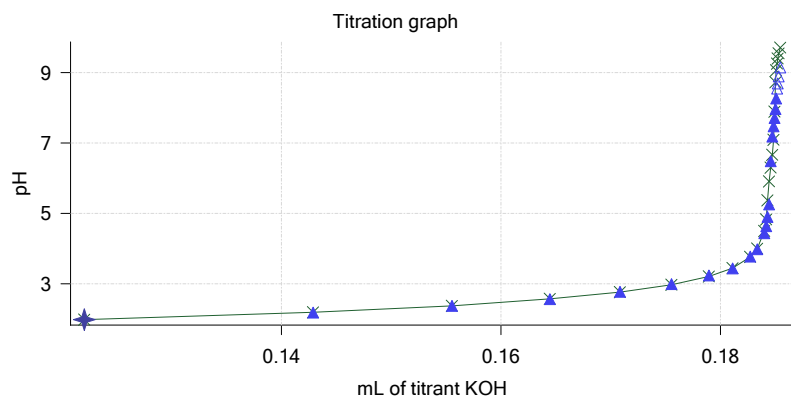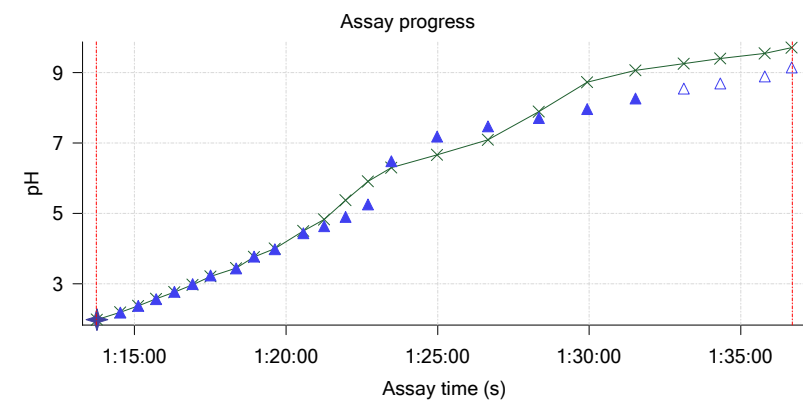| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:59.7	Initial pH = 4.07									
8:59.3	Data point 1	1.50000 mL	0.05094 mL	0.00682 mL	0.01999 mL	1.993	0.00166	0.09032	0.00027	10.0 s
9:45.6	Data point 2	1.50000 mL	0.05094 mL	0.02354 mL	0.01999 mL	2.195	-0.01016	0.27478	0.00096	10.0 s
10:21.2	Data point 3	1.50000 mL	0.05094 mL	0.03356 mL	0.01999 mL	2.380	-0.00393	0.49609	0.00028	10.0 s
10:56.8	Data point 4	1.50000 mL	0.05094 mL	0.04036 mL	0.01999 mL	2.583	-0.01061	0.30160	0.00095	10.0 s
11:32.3	Data point 5	1.50000 mL	0.05094 mL	0.04504 mL	0.01999 mL	2.791	-0.00615	0.53625	0.00041	10.0 s
12:07.9	Data point 6	1.50000 mL	0.05094 mL	0.04849 mL	0.01999 mL	2.973	-0.01184	0.89998	0.00062	10.0 s
12:43.3	Data point 7	1.50000 mL	0.05094 mL	0.05141 mL	0.01999 mL	3.161	-0.01641	0.89430	0.00086	10.0 s
13:18.8	Data point 8	1.50000 mL	0.05094 mL	0.05402 mL	0.01999 mL	3.380	-0.01816	0.97797	0.00091	10.0 s
13:54.4	Data point 9	1.50000 mL	0.05094 mL	0.05640 mL	0.01999 mL	3.621	-0.01999	0.98251	0.00100	11.0 s
14:41.2	Data point 10	1.50000 mL	0.05094 mL	0.05851 mL	0.01999 mL	3.854	-0.01872	0.92596	0.00096	11.5 s
15:18.1	Data point 11	1.50000 mL	0.05094 mL	0.06016 mL	0.01999 mL	4.021	-0.07914	0.99504	0.00392	Timed out at 59.5 s
16:43.6	Data point 12	1.50000 mL	0.05094 mL	0.06082 mL	0.01999 mL	4.014	-0.06809	0.99320	0.00337	Timed out at 59.5 s
18:09.0	Data point 13	1.50000 mL	0.05094 mL	0.06150 mL	0.01999 mL	4.183	-0.04322	0.98848	0.00215	Timed out at 59.5 s
19:34.3	Data point 14	1.50000 mL	0.05094 mL	0.06204 mL	0.01999 mL	4.377	-0.02931	0.97915	0.00146	Timed out at 59.5 s
20:59.7	Data point 15	1.50000 mL	0.05094 mL	0.06242 mL	0.01999 mL	4.584	-0.01998	0.99064	0.00099	48.5 s
22:13.6	Data point 16	1.50000 mL	0.05094 mL	0.06265 mL	0.01999 mL	4.745	-0.01777	0.91711	0.00092	54.0 s
23:33.1	Data point 17	1.50000 mL	0.05094 mL	0.06282 mL	0.01999 mL	4.902	-0.01909	0.98788	0.00095	46.5 s
24:50.2	Data point 18	1.50000 mL	0.05094 mL	0.06296 mL	0.01999 mL	5.053	-0.01967	0.95681	0.00099	57.5 s
26:13.2	Data point 19	1.50000 mL	0.05094 mL	0.06305 mL	0.01999 mL	5.207	-0.02130	0.95071	0.00108	Timed out at 59.5 s
27:43.7	Data point 20	1.50000 mL	0.05094 mL	0.06315 mL	0.01999 mL	5.387	-0.01948	0.92987	0.00100	57.5 s
29:11.7	Data point 21	1.50000 mL	0.05094 mL	0.06322 mL	0.01999 mL	5.573	-0.01912	0.95211	0.00097	59.0 s
30:41.3	Data point 22	1.50000 mL	0.05094 mL	0.06329 mL	0.01999 mL	5.905	-0.01889	0.90762	0.00098	51.5 s
32:03.4	Data point 23	1.50000 mL	0.05094 mL	0.06341 mL	0.01999 mL	6.675	-0.01975	0.98665	0.00098	57.0 s
33:31.0	Data point 24	1.50000 mL	0.05094 mL	0.06352 mL	0.01999 mL	7.182	-0.02923	0.95987	0.00147	Timed out at 59.5 s
35:06.7	Data point 25	1.50000 mL	0.05094 mL	0.06364 mL	0.01999 mL	7.640	-0.04416	0.98507	0.00220	Timed out at 59.5 s
36:42.3	Data point 26	1.50000 mL	0.05094 mL	0.06371 mL	0.01999 mL	7.920	-0.03822	0.98044	0.00191	Timed out at 59.5 s
38:17.9	Data point 27	1.50000 mL	0.05094 mL	0.06378 mL	0.01999 mL	8.284	-0.02815	0.97144	0.00141	Timed out at 59.5 s

Sample name: **M12_octanol**   Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-03013**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
39:53.6	Data point 28	1.50000 mL	0.05094 mL	0.06385 mL	0.01999 mL	8.653	-0.01851	0.94276	0.00094	56.5 s
41:25.8	Data point 29	1.50000 mL	0.05094 mL	0.06395 mL	0.01999 mL	8.880	-0.01941	0.93233	0.00099	43.5 s
42:40.0	Data point 30	1.50000 mL	0.05094 mL	0.06404 mL	0.01999 mL	9.109	-0.01865	0.94873	0.00095	37.5 s
44:11.2	Data point 31	1.50000 mL	0.10868 mL	0.06404 mL	0.05000 mL	1.992	-0.01464	0.98078	0.00073	10.0 s
44:57.5	Data point 32	1.50000 mL	0.10868 mL	0.08246 mL	0.05000 mL	2.204	-0.00623	0.39555	0.00049	10.0 s
45:33.2	Data point 33	1.50000 mL	0.10868 mL	0.09334 mL	0.05000 mL	2.395	0.00024	0.00175	0.00029	10.0 s
46:08.8	Data point 34	1.50000 mL	0.10868 mL	0.10075 mL	0.05000 mL	2.608	0.00510	0.08694	0.00085	10.0 s
46:44.4	Data point 35	1.50000 mL	0.10868 mL	0.10597 mL	0.05000 mL	2.821	-0.00756	0.57280	0.00049	10.0 s
47:19.9	Data point 36	1.50000 mL	0.10868 mL	0.10995 mL	0.05000 mL	3.049	-0.00595	0.80766	0.00033	10.5 s
47:56.0	Data point 37	1.50000 mL	0.10868 mL	0.11315 mL	0.05000 mL	3.262	-0.00544	0.73730	0.00031	10.5 s
48:32.0	Data point 38	1.50000 mL	0.10868 mL	0.11578 mL	0.05000 mL	3.477	-0.00488	0.14223	0.00064	10.0 s
49:07.5	Data point 39	1.50000 mL	0.10868 mL	0.11787 mL	0.05000 mL	3.757	-0.00502	0.11123	0.00074	10.5 s
49:53.8	Data point 40	1.50000 mL	0.10868 mL	0.11886 mL	0.05000 mL	3.930	-0.01303	0.75605	0.00074	10.5 s
50:29.7	Data point 41	1.50000 mL	0.10868 mL	0.11940 mL	0.05000 mL	4.156	-0.01560	0.85505	0.00083	12.0 s
51:17.4	Data point 42	1.50000 mL	0.10868 mL	0.12004 mL	0.05000 mL	4.490	-0.01911	0.93383	0.00098	46.0 s
52:28.8	Data point 43	1.50000 mL	0.10868 mL	0.12039 mL	0.05000 mL	4.732	-0.01804	0.90169	0.00094	52.0 s
53:51.5	Data point 44	1.50000 mL	0.10868 mL	0.12067 mL	0.05000 mL	5.082	-0.01877	0.92983	0.00096	48.5 s
55:10.7	Data point 45	1.50000 mL	0.10868 mL	0.12098 mL	0.05000 mL	6.196	-0.03857	0.98173	0.00192	Timed out at 59.5 s
56:41.2	Data point 46	1.50000 mL	0.10868 mL	0.12114 mL	0.05000 mL	6.798	-0.04966	0.98696	0.00247	Timed out at 59.5 s
58:11.7	Data point 47	1.50000 mL	0.10868 mL	0.12126 mL	0.05000 mL	7.026	-0.03315	0.95815	0.00167	Timed out at 59.5 s
59:42.2	Data point 48	1.50000 mL	0.10868 mL	0.12136 mL	0.05000 mL	7.152	-0.03446	0.98537	0.00171	Timed out at 59.5 s
1:01:17.8	Data point 49	1.50000 mL	0.10868 mL	0.12145 mL	0.05000 mL	7.458	-0.05118	0.98692	0.00254	Timed out at 59.5 s
1:02:53.4	Data point 50	1.50000 mL	0.10868 mL	0.12152 mL	0.05000 mL	7.749	-0.09026	0.98237	0.00450	Timed out at 59.5 s
1:04:29.0	Data point 51	1.50000 mL	0.10868 mL	0.12159 mL	0.05000 mL	7.874	-0.07009	0.98935	0.00348	Timed out at 59.5 s
1:06:04.6	Data point 52	1.50000 mL	0.10868 mL	0.12166 mL	0.05000 mL	8.208	-0.05709	0.99176	0.00283	Timed out at 59.5 s
1:07:45.4	Data point 53	1.50000 mL	0.10868 mL	0.12175 mL	0.05000 mL	8.485	-0.02993	0.97232	0.00150	Timed out at 59.5 s
1:09:26.2	Data point 54	1.50000 mL	0.10868 mL	0.12185 mL	0.05000 mL	8.684	-0.01638	0.69410	0.00097	39.5 s
1:10:41.4	Data point 55	1.50000 mL	0.10868 mL	0.12194 mL	0.05000 mL	8.903	-0.01932	0.91951	0.00099	53.5 s
1:12:05.4	Data point 56	1.50000 mL	0.10868 mL	0.12204 mL	0.05000 mL	9.050	-0.01983	0.98693	0.00099	37.0 s
1:13:45.4	Data point 57	1.50000 mL	0.17119 mL	0.12204 mL	0.25000 mL	1.982	-0.00868	0.51882	0.00059	10.0 s
1:14:31.7	Data point 58	1.50000 mL	0.17119 mL	0.14287 mL	0.25000 mL	2.187	-0.00313	0.29423	0.00028	10.0 s
1:15:07.5	Data point 59	1.50000 mL	0.17119 mL	0.15553 mL	0.25000 mL	2.372	0.00043	0.02077	0.00015	10.0 s
1:15:43.1	Data point 60	1.50000 mL	0.17119 mL	0.16446 mL	0.25000 mL	2.567	-0.00212	0.35123	0.00018	10.5 s
1:16:19.2	Data point 61	1.50000 mL	0.17119 mL	0.17084 mL	0.25000 mL	2.773	0.00623	0.11536	0.00091	10.0 s
1:16:54.7	Data point 62	1.50000 mL	0.17119 mL	0.17552 mL	0.25000 mL	2.992	-0.00796	0.85989	0.00042	10.0 s
1:17:30.2	Data point 63	1.50000 mL	0.17119 mL	0.17893 mL	0.25000 mL	3.240	-0.00517	0.42305	0.00039	10.0 s
1:18:21.2	Data point 64	1.50000 mL	0.17119 mL	0.18109 mL	0.25000 mL	3.441	0.00207	0.09593	0.00033	10.0 s
1:18:56.8	Data point 65	1.50000 mL	0.17119 mL	0.18271 mL	0.25000 mL	3.778	-0.00557	0.68049	0.00033	10.5 s
1:19:37.9	Data point 66	1.50000 mL	0.17119 mL	0.18335 mL	0.25000 mL	3.987	-0.00947	0.83986	0.00051	10.0 s
1:20:33.9	Data point 67	1.50000 mL	0.17119 mL	0.18398 mL	0.25000 mL	4.440	-0.01073	0.32598	0.00093	11.0 s
1:21:15.4	Data point 68	1.50000 mL	0.17119 mL	0.18415 mL	0.25000 mL	4.637	-0.01956	0.95178	0.00099	17.0 s
1:21:57.9	Data point 69	1.50000 mL	0.17119 mL	0.18429 mL	0.25000 mL	4.901	-0.01572	0.83949	0.00085	13.5 s
1:22:41.9	Data point 70	1.50000 mL	0.17119 mL	0.18443 mL	0.25000 mL	5.253	-0.01459	0.61037	0.00092	15.5 s
1:23:28.0	Data point 71	1.50000 mL	0.17119 mL	0.18457 mL	0.25000 mL	6.486	-0.02584	0.99076	0.00128	Timed out at 59.5 s
1:24:58.6	Data point 72	1.50000 mL	0.17119 mL	0.18471 mL	0.25000 mL	7.185	-0.06008	0.98340	0.00299	Timed out at 59.5 s

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:26:39.3	Data point 73	1.50000 mL	0.17119 mL	0.18483 mL	0.25000 mL	7.473	-0.04422	0.98321	0.00220	Timed out at 59.5 s
1:28:20.1	Data point 74	1.50000 mL	0.17119 mL	0.18493 mL	0.25000 mL	7.705	-0.05489	0.98906	0.00273	Timed out at 59.5 s
1:29:55.7	Data point 75	1.50000 mL	0.17119 mL	0.18499 mL	0.25000 mL	7.963	-0.05454	0.98638	0.00271	Timed out at 59.5 s
1:31:31.4	Data point 76	1.50000 mL	0.17119 mL	0.18507 mL	0.25000 mL	8.267	-0.04359	0.97797	0.00218	Timed out at 59.5 s
1:33:06.9	Data point 77	1.50000 mL	0.17119 mL	0.18514 mL	0.25000 mL	8.545	-0.01535	0.64494	0.00094	37.0 s
1:34:19.6	Data point 78	1.50000 mL	0.17119 mL	0.18521 mL	0.25000 mL	8.691	-0.01787	0.92709	0.00092	57.5 s
1:35:47.7	Data point 79	1.50000 mL	0.17119 mL	0.18530 mL	0.25000 mL	8.893	-0.01116	0.33380	0.00095	17.5 s
1:36:40.9	Data point 80	1.50000 mL	0.17119 mL	0.18544 mL	0.25000 mL	9.143	-0.01321	0.57777	0.00086	13.0 s
1:37:02.9	Assay volumes	1.50000 mL	0.17119 mL	0.18544 mL	0.25000 mL					

Sample name: **M12_octanol** Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-03013** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.030 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 4:33:34 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 4:33:34 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+6.23 mV		3/3/2018 4:34:02 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	6.6e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.8e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:38] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:07] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[5:53] Titrator arm moved to Titration position
[5:53] Argon flow rate set to 100
[5:53] Stirrer speed set to 10
[5:58] Automatically add 0.02000 mL of Octanol
[5:59] Dispensed 0.019991 mL of Octanol
[6:00] Initial pH = 4.07
[6:00] Iterative adjust 4.07 -> 2.00
[6:00] pH 4.07 -> 2.00
[6:01] Air gap released for Acid (0.5 M HCl)
[6:02] Dispensed 0.050941 mL of Acid (0.5 M HCl)
[6:07] Holding pH 2.00
[8:07] Stirrer speed set to 0
[8:07] Stirrer speed set to 50
[8:07] Iterative adjust 1.94 -> 2.00
[8:07] pH 1.94 -> 2.00
[8:08] Air gap released for Base (0.5 M KOH)
[8:09] Dispensed 0.006820 mL of Base (0.5 M KOH)
[8:59] Stirrer speed set to 0
[9:09] Datapoint id 1 collected
[9:09] Stirrer speed set to 50
[9:14] pH 2.00 -> 2.20
[9:14] Using cautious pH adjust
[9:15] Dispensed 0.007902 mL of Base (0.5 M KOH)
[9:20] Stepping pH = 2.08
[9:20] Dispensed 0.006985 mL of Base (0.5 M KOH)
[9:25] Stepping pH = 2.17
[9:25] Dispensed 0.001834 mL of Base (0.5 M KOH)
[9:30] Stepping pH = 2.20
[9:45] Stirrer speed set to 0
[9:55] Datapoint id 2 collected
[9:55] Charge balance equation is out by -5.8%
[9:55] Stirrer speed set to 50

Sample name: **M12_octanol**   Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-03013**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[10:01] pH 2.20 -> 2.40
[10:01] Using charge balance adjust
[10:01] Dispensed 0.010019 mL of Base (0.5 M KOH)
[10:21] Stirrer speed set to 0
[10:31] Datapoint id 3 collected
[10:31] Charge balance equation is out by -11.0%
[10:31] Stirrer speed set to 50
[10:36] pH 2.39 -> 2.59
[10:36] Using charge balance adjust
[10:36] Dispensed 0.006797 mL of Base (0.5 M KOH)
[10:57] Stirrer speed set to 0
[11:07] Datapoint id 4 collected
[11:07] Charge balance equation is out by -2.1%
[11:07] Stirrer speed set to 50
[11:12] pH 2.59 -> 2.79
[11:12] Using charge balance adjust
[11:12] Dispensed 0.004680 mL of Base (0.5 M KOH)
[11:32] Stirrer speed set to 0
[11:42] Datapoint id 5 collected
[11:42] Charge balance equation is out by 0.9%
[11:42] Stirrer speed set to 50
[11:47] pH 2.80 -> 3.00
[11:47] Using charge balance adjust
[11:48] Dispensed 0.003457 mL of Base (0.5 M KOH)
[12:08] Stirrer speed set to 0
[12:18] Datapoint id 6 collected
[12:18] Charge balance equation is out by -12.7%
[12:18] Stirrer speed set to 50
[12:23] pH 2.98 -> 3.18
[12:23] Using charge balance adjust
[12:23] Dispensed 0.002916 mL of Base (0.5 M KOH)
[12:43] Stirrer speed set to 0
[12:53] Datapoint id 7 collected
[12:53] Charge balance equation is out by -8.1%
[12:53] Stirrer speed set to 50
[12:58] pH 3.17 -> 3.37
[12:58] Using charge balance adjust
[12:58] Dispensed 0.002611 mL of Base (0.5 M KOH)
[13:19] Stirrer speed set to 0
[13:29] Datapoint id 8 collected
[13:29] Charge balance equation is out by 7.3%
[13:29] Stirrer speed set to 50
[13:34] pH 3.38 -> 3.58
[13:34] Using charge balance adjust
[13:34] Dispensed 0.002375 mL of Base (0.5 M KOH)
[13:54] Stirrer speed set to 0
[14:05] Datapoint id 9 collected
[14:05] Charge balance equation is out by 18.9%
[14:05] Stirrer speed set to 50
[14:10] pH 3.62 -> 3.82
[14:10] Using cautious pH adjust
[14:10] Dispensed 0.001035 mL of Base (0.5 M KOH)
[14:16] Stepping pH = 3.77
[14:16] Dispensed 0.000329 mL of Base (0.5 M KOH)
[14:21] Stepping pH = 3.77
[14:21] Dispensed 0.000753 mL of Base (0.5 M KOH)
[14:26] Stepping pH = 3.89
[14:41] Stirrer speed set to 0
[14:53] Datapoint id 10 collected

Sample name: **M12_octanol** Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-03013** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[14:53] Charge balance equation is out by -3.0%
[14:53] Stirrer speed set to 50
[14:58] pH 3.86 -> 4.06
[14:58] Using charge balance adjust
[14:58] Dispensed 0.001646 mL of Base (0.5 M KOH)
[15:18] Stirrer speed set to 0
[16:18] Datapoint id 11 collected
[16:18] Charge balance equation is out by -20.9%
[16:18] Stirrer speed set to 50
[16:23] pH 4.02 -> 4.22
[16:23] Using cautious pH adjust
[16:23] Dispensed 0.000659 mL of Base (0.5 M KOH)
[16:28] Stepping pH = 4.23
[16:43] Stirrer speed set to 0
[17:43] Datapoint id 12 collected
[17:43] Charge balance equation is out by 50.0%
[17:43] Stirrer speed set to 50
[17:49] pH 4.01 -> 4.21
[17:49] Using cautious pH adjust
[17:49] Dispensed 0.000682 mL of Base (0.5 M KOH)
[17:54] Stepping pH = 4.38
[18:09] Stirrer speed set to 0
[19:09] Datapoint id 13 collected
[19:09] Charge balance equation is out by 50.0%
[19:09] Stirrer speed set to 50
[19:14] pH 4.18 -> 4.38
[19:14] Using cautious pH adjust
[19:14] Dispensed 0.000541 mL of Base (0.5 M KOH)
[19:19] Stepping pH = 4.58
[19:34] Stirrer speed set to 0
[20:34] Datapoint id 14 collected
[20:34] Charge balance equation is out by 50.0%
[20:34] Stirrer speed set to 50
[20:39] pH 4.38 -> 4.58
[20:39] Using cautious pH adjust
[20:39] Dispensed 0.000376 mL of Base (0.5 M KOH)
[20:44] Stepping pH = 4.77
[21:00] Stirrer speed set to 0
[21:48] Datapoint id 15 collected
[21:48] Charge balance equation is out by 50.0%
[21:48] Stirrer speed set to 50
[21:53] pH 4.61 -> 4.81
[21:53] Using cautious pH adjust
[21:53] Dispensed 0.000235 mL of Base (0.5 M KOH)
[21:58] Stepping pH = 4.90
[22:14] Stirrer speed set to 0
[23:08] Datapoint id 16 collected
[23:08] Charge balance equation is out by 50.0%
[23:08] Stirrer speed set to 50
[23:13] pH 4.77 -> 4.97
[23:13] Using cautious pH adjust
[23:13] Dispensed 0.000165 mL of Base (0.5 M KOH)
[23:18] Stepping pH = 5.01
[23:33] Stirrer speed set to 0
[24:20] Datapoint id 17 collected
[24:20] Charge balance equation is out by 50.0%
[24:20] Stirrer speed set to 50
[24:25] pH 4.93 -> 5.13
[24:25] Using cautious pH adjust

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[24:25] Dispensed 0.000118 mL of Base (0.5 M KOH)
[24:30] Stepping pH = 5.12
[24:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:35] Stepping pH = 5.14
[24:50] Stirrer speed set to 0
[25:48] Datapoint id 18 collected
[25:48] Charge balance equation is out by 42.0%
[25:48] Stirrer speed set to 50
[25:53] pH 5.09 -> 5.29
[25:53] Using cautious pH adjust
[25:53] Dispensed 0.000094 mL of Base (0.5 M KOH)
[25:58] Stepping pH = 5.30
[26:13] Stirrer speed set to 0
[27:13] Datapoint id 19 collected
[27:13] Charge balance equation is out by 50.0%
[27:13] Stirrer speed set to 50
[27:18] pH 5.22 -> 5.42
[27:18] Using cautious pH adjust
[27:18] Dispensed 0.000071 mL of Base (0.5 M KOH)
[27:23] Stepping pH = 5.35
[27:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:28] Stepping pH = 5.44
[27:44] Stirrer speed set to 0
[28:41] Datapoint id 20 collected
[28:41] Charge balance equation is out by 30.4%
[28:41] Stirrer speed set to 50
[28:46] pH 5.39 -> 5.59
[28:46] Using cautious pH adjust
[28:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[28:51] Stepping pH = 5.50
[28:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:56] Stepping pH = 5.60
[29:12] Stirrer speed set to 0
[30:11] Datapoint id 21 collected
[30:11] Charge balance equation is out by 20.0%
[30:11] Stirrer speed set to 50
[30:16] pH 5.58 -> 5.78
[30:16] Using cautious pH adjust
[30:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[30:21] Stepping pH = 5.73
[30:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[30:26] Stepping pH = 5.90
[30:41] Stirrer speed set to 0
[31:33] Datapoint id 22 collected
[31:33] Charge balance equation is out by 25.8%
[31:33] Stirrer speed set to 50
[31:38] pH 5.90 -> 6.10
[31:38] Using cautious pH adjust
[31:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:43] Stepping pH = 5.91
[31:43] Dispensed 0.000094 mL of Base (0.5 M KOH)
[31:48] Stepping pH = 6.63
[32:03] Stirrer speed set to 0
[33:00] Datapoint id 23 collected
[33:00] Charge balance equation is out by -90.2%
[33:00] Stirrer speed set to 50
[33:06] pH 6.63 -> 6.83
[33:06] Using cautious pH adjust
[33:06] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[33:11] Stepping pH = 6.61
[33:11] Dispensed 0.000094 mL of Base (0.5 M KOH)
[33:16] Stepping pH = 7.08
[33:31] Stirrer speed set to 0
[34:31] Datapoint id 24 collected
[34:31] Charge balance equation is out by -229.9%
[34:31] Stirrer speed set to 50
[34:36] pH 7.12 -> 7.32
[34:36] Using cautious pH adjust
[34:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:41] Stepping pH = 7.09
[34:41] Dispensed 0.000047 mL of Base (0.5 M KOH)
[34:46] Stepping pH = 7.18
[34:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[34:51] Stepping pH = 7.57
[35:07] Stirrer speed set to 0
[36:07] Datapoint id 25 collected
[36:07] Charge balance equation is out by -576.8%
[36:07] Stirrer speed set to 50
[36:12] pH 7.58 -> 7.78
[36:12] Using cautious pH adjust
[36:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:17] Stepping pH = 7.57
[36:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:22] Stepping pH = 7.63
[36:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:27] Stepping pH = 7.82
[36:42] Stirrer speed set to 0
[37:42] Datapoint id 26 collected
[37:42] Charge balance equation is out by -808.4%
[37:42] Stirrer speed set to 50
[37:47] pH 7.85 -> 8.05
[37:47] Using cautious pH adjust
[37:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:52] Stepping pH = 7.82
[37:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:58] Stepping pH = 7.89
[37:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:03] Stepping pH = 8.14
[38:18] Stirrer speed set to 0
[39:18] Datapoint id 27 collected
[39:18] Charge balance equation is out by -902.2%
[39:18] Stirrer speed set to 50
[39:23] pH 8.29 -> 8.49
[39:23] Using cautious pH adjust
[39:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:28] Stepping pH = 8.33
[39:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:33] Stepping pH = 8.43
[39:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:38] Stepping pH = 8.64
[39:53] Stirrer speed set to 0
[40:50] Datapoint id 28 collected
[40:50] Charge balance equation is out by -511.3%
[40:50] Stirrer speed set to 50
[40:55] pH 8.63 -> 8.83
[40:55] Using cautious pH adjust
[40:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:00] Stepping pH = 8.59

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[41:00] Dispensed 0.000047 mL of Base (0.5 M KOH)
[41:05] Stepping pH = 8.78
[41:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:11] Stepping pH = 8.93
[41:26] Stirrer speed set to 0
[42:09] Datapoint id 29 collected
[42:09] Charge balance equation is out by -393.5%
[42:09] Stirrer speed set to 50
[42:14] pH 8.86 -> 9.05
[42:14] Using cautious pH adjust
[42:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:20] Stepping pH = 8.86
[42:20] Dispensed 0.000071 mL of Base (0.5 M KOH)
[42:25] Stepping pH = 9.12
[42:40] Stirrer speed set to 0
[43:17] Datapoint id 30 collected
[43:17] Charge balance equation is out by -226.3%
[43:17] Titration 2 of 3
[43:17] Adding initial titrants
[43:17] Automatically add 0.03000 mL of Octanol
[43:18] Dispensed 0.030009 mL of Octanol
[43:18] Stirrer speed set to 10
[43:19] Stirrer speed set to 55
[43:19] Iterative adjust 9.11 -> 2.00
[43:19] pH 9.11 -> 2.00
[43:21] Dispensed 0.057738 mL of Acid (0.5 M HCl)
[44:11] Stirrer speed set to 0
[44:21] Datapoint id 31 collected
[44:21] Stirrer speed set to 55
[44:26] pH 2.00 -> 2.20
[44:26] Using cautious pH adjust
[44:27] Dispensed 0.008537 mL of Base (0.5 M KOH)
[44:32] Stepping pH = 2.08
[44:32] Dispensed 0.007855 mL of Base (0.5 M KOH)
[44:37] Stepping pH = 2.17
[44:37] Dispensed 0.002023 mL of Base (0.5 M KOH)
[44:42] Stepping pH = 2.21
[44:57] Stirrer speed set to 0
[45:07] Datapoint id 32 collected
[45:07] Charge balance equation is out by -7.9%
[45:07] Stirrer speed set to 55
[45:13] pH 2.21 -> 2.41
[45:13] Using charge balance adjust
[45:13] Dispensed 0.010889 mL of Base (0.5 M KOH)
[45:33] Stirrer speed set to 0
[45:43] Datapoint id 33 collected
[45:43] Charge balance equation is out by -6.8%
[45:43] Stirrer speed set to 55
[45:48] pH 2.40 -> 2.60
[45:48] Using charge balance adjust
[45:48] Dispensed 0.007408 mL of Base (0.5 M KOH)
[46:09] Stirrer speed set to 0
[46:19] Datapoint id 34 collected
[46:19] Charge balance equation is out by 2.4%
[46:19] Stirrer speed set to 55
[46:24] pH 2.61 -> 2.81
[46:24] Using charge balance adjust
[46:24] Dispensed 0.005221 mL of Base (0.5 M KOH)
[46:44] Stirrer speed set to 0

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[46:54] Datapoint id 35 collected
[46:54] Charge balance equation is out by 3.1%
[46:54] Stirrer speed set to 55
[46:59] pH 2.83 -> 3.03
[46:59] Using charge balance adjust
[47:00] Dispensed 0.003975 mL of Base (0.5 M KOH)
[47:20] Stirrer speed set to 0
[47:30] Datapoint id 36 collected
[47:30] Charge balance equation is out by 11.3%
[47:30] Stirrer speed set to 55
[47:35] pH 3.05 -> 3.25
[47:35] Using charge balance adjust
[47:36] Dispensed 0.003198 mL of Base (0.5 M KOH)
[47:56] Stirrer speed set to 0
[48:06] Datapoint id 37 collected
[48:06] Charge balance equation is out by 5.8%
[48:06] Stirrer speed set to 55
[48:12] pH 3.26 -> 3.46
[48:12] Using charge balance adjust
[48:12] Dispensed 0.002634 mL of Base (0.5 M KOH)
[48:32] Stirrer speed set to 0
[48:42] Datapoint id 38 collected
[48:42] Charge balance equation is out by 8.2%
[48:42] Stirrer speed set to 55
[48:47] pH 3.48 -> 3.68
[48:47] Using charge balance adjust
[48:47] Dispensed 0.002093 mL of Base (0.5 M KOH)
[49:07] Stirrer speed set to 0
[49:18] Datapoint id 39 collected
[49:18] Charge balance equation is out by 39.2%
[49:18] Stirrer speed set to 55
[49:23] pH 3.74 -> 3.94
[49:23] Using cautious pH adjust
[49:23] Dispensed 0.000729 mL of Base (0.5 M KOH)
[49:28] Stepping pH = 3.89
[49:28] Dispensed 0.000188 mL of Base (0.5 M KOH)
[49:33] Stepping pH = 3.93
[49:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[49:39] Stepping pH = 3.94
[49:54] Stirrer speed set to 0
[50:04] Datapoint id 40 collected
[50:04] Charge balance equation is out by 32.9%
[50:04] Stirrer speed set to 55
[50:09] pH 3.93 -> 4.13
[50:09] Using cautious pH adjust
[50:09] Dispensed 0.000541 mL of Base (0.5 M KOH)
[50:14] Stepping pH = 4.19
[50:30] Stirrer speed set to 0
[50:42] Datapoint id 41 collected
[50:42] Charge balance equation is out by 50.0%
[50:42] Stirrer speed set to 55
[50:47] pH 4.16 -> 4.36
[50:47] Using cautious pH adjust
[50:47] Dispensed 0.000353 mL of Base (0.5 M KOH)
[50:52] Stepping pH = 4.33
[50:52] Dispensed 0.000047 mL of Base (0.5 M KOH)
[50:57] Stepping pH = 4.33
[50:57] Dispensed 0.000235 mL of Base (0.5 M KOH)
[51:02] Stepping pH = 4.58

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[51:17] Stirrer speed set to 0
[52:03] Datapoint id 42 collected
[52:03] Charge balance equation is out by 10.7%
[52:03] Stirrer speed set to 55
[52:08] pH 4.50 -> 4.70
[52:08] Using charge balance adjust
[52:09] Dispensed 0.000353 mL of Base (0.5 M KOH)
[52:29] Stirrer speed set to 0
[53:21] Datapoint id 43 collected
[53:21] Charge balance equation is out by 15.6%
[53:21] Stirrer speed set to 55
[53:26] pH 4.76 -> 4.96
[53:26] Using cautious pH adjust
[53:26] Dispensed 0.000094 mL of Base (0.5 M KOH)
[53:31] Stepping pH = 4.80
[53:31] Dispensed 0.000188 mL of Base (0.5 M KOH)
[53:36] Stepping pH = 5.29
[53:51] Stirrer speed set to 0
[54:40] Datapoint id 44 collected
[54:40] Charge balance equation is out by -45.8%
[54:40] Stirrer speed set to 55
[54:45] pH 5.11 -> 5.31
[54:45] Using cautious pH adjust
[54:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[54:50] Stepping pH = 5.10
[54:50] Dispensed 0.000259 mL of Base (0.5 M KOH)
[54:55] Stepping pH = 6.40
[55:11] Stirrer speed set to 0
[56:11] Datapoint id 45 collected
[56:11] Charge balance equation is out by -213.5%
[56:11] Stirrer speed set to 55
[56:16] pH 6.18 -> 6.38
[56:16] Using cautious pH adjust
[56:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:21] Stepping pH = 6.15
[56:21] Dispensed 0.000141 mL of Base (0.5 M KOH)
[56:26] Stepping pH = 6.88
[56:41] Stirrer speed set to 0
[57:41] Datapoint id 46 collected
[57:41] Charge balance equation is out by -239.0%
[57:41] Stirrer speed set to 55
[57:46] pH 6.75 -> 6.95
[57:46] Using cautious pH adjust
[57:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:51] Stepping pH = 6.70
[57:51] Dispensed 0.000094 mL of Base (0.5 M KOH)
[57:56] Stepping pH = 7.05
[58:12] Stirrer speed set to 0
[59:12] Datapoint id 47 collected
[59:12] Charge balance equation is out by -295.8%
[59:12] Stirrer speed set to 55
[59:17] pH 6.96 -> 7.16
[59:17] Using cautious pH adjust
[59:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:22] Stepping pH = 6.90
[59:22] Dispensed 0.000071 mL of Base (0.5 M KOH)
[59:27] Stepping pH = 7.18
[59:42] Stirrer speed set to 0
[1:00:42] Datapoint id 48 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:00:42] Charge balance equation is out by -327.5%
[1:00:42] Stirrer speed set to 55
[1:00:47] pH 7.10 -> 7.30
[1:00:47] Using cautious pH adjust
[1:00:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:52] Stepping pH = 7.09
[1:00:52] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:00:57] Stepping pH = 7.27
[1:00:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:03] Stepping pH = 7.45
[1:01:18] Stirrer speed set to 0
[1:02:18] Datapoint id 49 collected
[1:02:18] Charge balance equation is out by -423.0%
[1:02:18] Stirrer speed set to 55
[1:02:23] pH 7.49 -> 7.69
[1:02:23] Using cautious pH adjust
[1:02:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:28] Stepping pH = 7.52
[1:02:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:33] Stepping pH = 7.64
[1:02:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:38] Stepping pH = 7.87
[1:02:53] Stirrer speed set to 0
[1:03:53] Datapoint id 50 collected
[1:03:53] Charge balance equation is out by -597.1%
[1:03:53] Stirrer speed set to 55
[1:03:58] pH 7.64 -> 7.84
[1:03:58] Using cautious pH adjust
[1:03:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:04] Stepping pH = 7.62
[1:04:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:09] Stepping pH = 7.72
[1:04:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:14] Stepping pH = 7.86
[1:04:29] Stirrer speed set to 0
[1:05:29] Datapoint id 51 collected
[1:05:29] Charge balance equation is out by -723.3%
[1:05:29] Stirrer speed set to 55
[1:05:34] pH 7.76 -> 7.96
[1:05:34] Using cautious pH adjust
[1:05:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:39] Stepping pH = 7.75
[1:05:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:44] Stepping pH = 7.91
[1:05:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:49] Stepping pH = 8.15
[1:06:05] Stirrer speed set to 0
[1:07:05] Datapoint id 52 collected
[1:07:05] Charge balance equation is out by -787.5%
[1:07:05] Stirrer speed set to 55
[1:07:10] pH 8.14 -> 8.34
[1:07:10] Using cautious pH adjust
[1:07:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:15] Stepping pH = 8.11
[1:07:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:20] Stepping pH = 8.17
[1:07:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:25] Stepping pH = 8.30
[1:07:25] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**   Experiment start time: **3/3/2018 4:33:34 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-03013**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[1:07:30] Stepping pH = 8.46
[1:07:45] Stirrer speed set to 0
[1:08:45] Datapoint id 53 collected
[1:08:45] Charge balance equation is out by -1,072.2%
[1:08:45] Stirrer speed set to 55
[1:08:50] pH 8.40 -> 8.60
[1:08:50] Using cautious pH adjust
[1:08:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:56] Stepping pH = 8.40
[1:08:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:01] Stepping pH = 8.48
[1:09:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:06] Stepping pH = 8.59
[1:09:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:11] Stepping pH = 8.69
[1:09:26] Stirrer speed set to 0
[1:10:06] Datapoint id 54 collected
[1:10:06] Charge balance equation is out by -722.4%
[1:10:06] Stirrer speed set to 55
[1:10:11] pH 8.66 -> 8.86
[1:10:11] Using cautious pH adjust
[1:10:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:16] Stepping pH = 8.66
[1:10:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:21] Stepping pH = 8.72
[1:10:21] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:10:26] Stepping pH = 8.90
[1:10:41] Stirrer speed set to 0
[1:11:35] Datapoint id 55 collected
[1:11:35] Charge balance equation is out by -320.7%
[1:11:35] Stirrer speed set to 55
[1:11:40] pH 8.88 -> 9.05
[1:11:40] Using cautious pH adjust
[1:11:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:11:45] Stepping pH = 8.87
[1:11:45] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:11:50] Stepping pH = 9.03
[1:12:05] Stirrer speed set to 0
[1:12:42] Datapoint id 56 collected
[1:12:42] Charge balance equation is out by -231.7%
[1:12:42] Titration 3 of 3
[1:12:42] Adding initial titrants
[1:12:42] Automatically add 0.20000 mL of Octanol
[1:12:47] Dispensed 0.200000 mL of Octanol
[1:12:47] Stirrer speed set to 10
[1:12:48] Stirrer speed set to 60
[1:12:48] Iterative adjust 9.05 -> 2.00
[1:12:48] pH 9.05 -> 2.00
[1:12:50] Dispensed 0.059784 mL of Acid (0.5 M HCl)
[1:12:55] pH 2.02 -> 2.00
[1:12:55] Dispensed 0.002728 mL of Acid (0.5 M HCl)
[1:13:45] Stirrer speed set to 0
[1:13:55] Datapoint id 57 collected
[1:13:55] Stirrer speed set to 60
[1:14:00] pH 1.99 -> 2.19
[1:14:00] Using cautious pH adjust
[1:14:01] Dispensed 0.009619 mL of Base (0.5 M KOH)
[1:14:06] Stepping pH = 2.07
[1:14:06] Dispensed 0.008843 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
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Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:14:11] Stepping pH = 2.16
[1:14:11] Dispensed 0.002375 mL of Base (0.5 M KOH)
[1:14:16] Stepping pH = 2.19
[1:14:32] Stirrer speed set to 0
[1:14:42] Datapoint id 58 collected
[1:14:42] Charge balance equation is out by -8.3%
[1:14:42] Stirrer speed set to 60
[1:14:47] pH 2.19 -> 2.39
[1:14:47] Using charge balance adjust
[1:14:47] Dispensed 0.012653 mL of Base (0.5 M KOH)
[1:15:07] Stirrer speed set to 0
[1:15:17] Datapoint id 59 collected
[1:15:17] Charge balance equation is out by -9.4%
[1:15:17] Stirrer speed set to 60
[1:15:22] pH 2.37 -> 2.57
[1:15:22] Using charge balance adjust
[1:15:23] Dispensed 0.008937 mL of Base (0.5 M KOH)
[1:15:43] Stirrer speed set to 0
[1:15:53] Datapoint id 60 collected
[1:15:53] Charge balance equation is out by -3.8%
[1:15:53] Stirrer speed set to 60
[1:15:59] pH 2.57 -> 2.77
[1:15:59] Using charge balance adjust
[1:15:59] Dispensed 0.006373 mL of Base (0.5 M KOH)
[1:16:19] Stirrer speed set to 0
[1:16:29] Datapoint id 61 collected
[1:16:29] Charge balance equation is out by -0.8%
[1:16:29] Stirrer speed set to 60
[1:16:34] pH 2.78 -> 2.98
[1:16:34] Using charge balance adjust
[1:16:34] Dispensed 0.004680 mL of Base (0.5 M KOH)
[1:16:55] Stirrer speed set to 0
[1:17:05] Datapoint id 62 collected
[1:17:05] Charge balance equation is out by 5.8%
[1:17:05] Stirrer speed set to 60
[1:17:10] pH 3.00 -> 3.20
[1:17:10] Using charge balance adjust
[1:17:10] Dispensed 0.003410 mL of Base (0.5 M KOH)
[1:17:30] Stirrer speed set to 0
[1:17:40] Datapoint id 63 collected
[1:17:40] Charge balance equation is out by 22.0%
[1:17:40] Stirrer speed set to 60
[1:17:45] pH 3.24 -> 3.44
[1:17:45] Using cautious pH adjust
[1:17:45] Dispensed 0.001152 mL of Base (0.5 M KOH)
[1:17:50] Stepping pH = 3.35
[1:17:51] Dispensed 0.000706 mL of Base (0.5 M KOH)
[1:17:56] Stepping pH = 3.43
[1:17:56] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:18:01] Stepping pH = 3.43
[1:18:01] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:18:06] Stepping pH = 3.44
[1:18:21] Stirrer speed set to 0
[1:18:31] Datapoint id 64 collected
[1:18:31] Charge balance equation is out by 6.4%
[1:18:31] Stirrer speed set to 60
[1:18:36] pH 3.45 -> 3.65
[1:18:36] Using charge balance adjust
[1:18:36] Dispensed 0.001623 mL of Base (0.5 M KOH)

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03013**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03013_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:18:57] Stirrer speed set to 0
[1:19:07] Datapoint id 65 collected
[1:19:07] Charge balance equation is out by 64.7%
[1:19:07] Stirrer speed set to 60
[1:19:12] pH 3.79 -> 3.99
[1:19:12] Using cautious pH adjust
[1:19:12] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:19:17] Stepping pH = 3.90
[1:19:18] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:19:23] Stepping pH = 3.99
[1:19:38] Stirrer speed set to 0
[1:19:48] Datapoint id 66 collected
[1:19:48] Charge balance equation is out by 25.8%
[1:19:48] Stirrer speed set to 60
[1:19:53] pH 4.00 -> 4.20
[1:19:53] Using cautious pH adjust
[1:19:53] Dispensed 0.000282 mL of Base (0.5 M KOH)
[1:19:58] Stepping pH = 4.15
[1:19:58] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:20:03] Stepping pH = 4.17
[1:20:03] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:20:08] Stepping pH = 4.18
[1:20:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:14] Stepping pH = 4.18
[1:20:14] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:20:19] Stepping pH = 4.45
[1:20:34] Stirrer speed set to 0
[1:20:45] Datapoint id 67 collected
[1:20:45] Charge balance equation is out by -17.7%
[1:20:45] Stirrer speed set to 60
[1:20:50] pH 4.46 -> 4.66
[1:20:50] Using cautious pH adjust
[1:20:50] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:20:55] Stepping pH = 4.56
[1:20:55] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:21:00] Stepping pH = 4.66
[1:21:15] Stirrer speed set to 0
[1:21:32] Datapoint id 68 collected
[1:21:32] Charge balance equation is out by 13.8%
[1:21:32] Stirrer speed set to 60
[1:21:37] pH 4.64 -> 4.84
[1:21:37] Using charge balance adjust
[1:21:38] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:21:58] Stirrer speed set to 0
[1:22:11] Datapoint id 69 collected
[1:22:11] Charge balance equation is out by 29.9%
[1:22:11] Stirrer speed set to 60
[1:22:16] pH 4.94 -> 5.14
[1:22:16] Using cautious pH adjust
[1:22:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:22:22] Stepping pH = 4.95
[1:22:22] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:22:27] Stepping pH = 5.40
[1:22:42] Stirrer speed set to 0
[1:22:57] Datapoint id 70 collected
[1:22:57] Charge balance equation is out by -92.0%
[1:22:57] Stirrer speed set to 60
[1:23:02] pH 5.25 -> 5.45
[1:23:02] Using cautious pH adjust

Sample name: **M12_octanol**
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Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:23:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:08] Stepping pH = 5.23
[1:23:08] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:23:13] Stepping pH = 6.55
[1:23:28] Stirrer speed set to 0
[1:24:28] Datapoint id 71 collected
[1:24:28] Charge balance equation is out by -224.6%
[1:24:28] Stirrer speed set to 60
[1:24:33] pH 6.43 -> 6.63
[1:24:33] Using cautious pH adjust
[1:24:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:24:38] Stepping pH = 6.42
[1:24:38] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:24:43] Stepping pH = 7.17
[1:24:58] Stirrer speed set to 0
[1:25:59] Datapoint id 72 collected
[1:25:59] Charge balance equation is out by -216.2%
[1:25:59] Stirrer speed set to 60
[1:26:04] pH 7.15 -> 7.35
[1:26:04] Using cautious pH adjust
[1:26:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:09] Stepping pH = 7.17
[1:26:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:14] Stepping pH = 7.23
[1:26:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:19] Stepping pH = 7.25
[1:26:19] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:26:24] Stepping pH = 7.50
[1:26:39] Stirrer speed set to 0
[1:27:39] Datapoint id 73 collected
[1:27:39] Charge balance equation is out by -583.7%
[1:27:39] Stirrer speed set to 60
[1:27:44] pH 7.42 -> 7.62
[1:27:44] Using cautious pH adjust
[1:27:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:27:49] Stepping pH = 7.42
[1:27:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:27:55] Stepping pH = 7.46
[1:27:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:00] Stepping pH = 7.58
[1:28:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:05] Stepping pH = 7.75
[1:28:20] Stirrer speed set to 0
[1:29:20] Datapoint id 74 collected
[1:29:20] Charge balance equation is out by -640.0%
[1:29:20] Stirrer speed set to 60
[1:29:25] pH 7.76 -> 7.96
[1:29:25] Using cautious pH adjust
[1:29:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:30] Stepping pH = 7.85
[1:29:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:35] Stepping pH = 7.93
[1:29:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:40] Stepping pH = 8.03
[1:29:56] Stirrer speed set to 0
[1:30:56] Datapoint id 75 collected
[1:30:56] Charge balance equation is out by -626.4%
[1:30:56] Stirrer speed set to 60
[1:31:01] pH 7.91 -> 8.11

Sample name: **M12_octanol**
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Experiment start time: **3/3/2018 4:33:34 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:31:01] Using cautious pH adjust
[1:31:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:06] Stepping pH = 7.96
[1:31:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:11] Stepping pH = 8.09
[1:31:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:16] Stepping pH = 8.32
[1:31:31] Stirrer speed set to 0
[1:32:31] Datapoint id 76 collected
[1:32:31] Charge balance equation is out by -645.7%
[1:32:31] Stirrer speed set to 60
[1:32:36] pH 8.27 -> 8.47
[1:32:36] Using cautious pH adjust
[1:32:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:41] Stepping pH = 8.32
[1:32:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:47] Stepping pH = 8.46
[1:32:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:52] Stepping pH = 8.58
[1:33:07] Stirrer speed set to 0
[1:33:44] Datapoint id 77 collected
[1:33:44] Charge balance equation is out by -426.1%
[1:33:44] Stirrer speed set to 60
[1:33:49] pH 8.51 -> 8.71
[1:33:49] Using cautious pH adjust
[1:33:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:33:54] Stepping pH = 8.53
[1:33:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:33:59] Stepping pH = 8.59
[1:33:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:04] Stepping pH = 8.72
[1:34:19] Stirrer speed set to 0
[1:35:17] Datapoint id 78 collected
[1:35:17] Charge balance equation is out by -316.1%
[1:35:17] Stirrer speed set to 60
[1:35:22] pH 8.65 -> 8.85
[1:35:22] Using cautious pH adjust
[1:35:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:35:27] Stepping pH = 8.63
[1:35:27] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:35:32] Stepping pH = 8.91
[1:35:48] Stirrer speed set to 0
[1:36:05] Datapoint id 79 collected
[1:36:05] Charge balance equation is out by -257.2%
[1:36:05] Stirrer speed set to 60
[1:36:10] pH 8.90 -> 9.05
[1:36:10] Using cautious pH adjust
[1:36:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:36:15] Stepping pH = 8.92
[1:36:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:36:20] Stepping pH = 8.94
[1:36:21] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:36:26] Stepping pH = 9.14
[1:36:41] Stirrer speed set to 0
[1:36:54] Datapoint id 80 collected
[1:36:54] Charge balance equation is out by -421.1%
[1:36:54] Argon flow rate set to 0
[1:36:58] Titrator arm moved over Titration position